ELASTIC SCATTERING AND POLARIZATION OF ELECTRONS BY ATOM IN SECOND BORN APPROXIMATION

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ABSTRACT. In the present paper, the differential cross section of scattering and the asymmetry after double scattering for electrons of energy 121 kev by screened field of the gold atom have been calculated by the Born method in second approximation, the theoretical findings have been compared with the exact results obtained by numerical computation. The comparison allows us to re-examine the degree of validity of the Born method in scattering process. It is found that the second Born approximation gives fairly good results for scattering cross section of 121 kev electrons, but for polarization effect, the second approximation is inadequate.

INTRODUCTION

In recent years, the study of scattering and polarization of electrons in the field of a heavy atom has assumed importance because of the relevancy of the latter to β-decay interactions theories. There are two main difficulties, one of them is the choice of a suitable representation of the screened field surrounding the atomic nucleus and the other is the limited range within which the analytical methods are valid. Because of the latter difficulty, recourse to numerical computation is now almost a common practice. Apart from mathematical nicety the analytical method often allows us to probe the problem step by step. With that in view we have calculated by second Born approximation the cross section of scattering and the consequent polarization of electrons in the field of the gold atom.

The nucleus of a heavy atom is surrounded by an electronic cloud; the effective field of such a system is usually given by the Thomas-Femi or Hartree-Fock method; in our calculations we have taken the 'two term field' of Mohr and Tassie (1954) which reproduces the Hartree field for gold very well.

Bartlet and Welton (1941) have calculated the cross section of scattering of electrons of energy 100 kev and 230 kev in the screened field of mercury atom by three methods : (1) Integration with differential analyser, (2) W. K. B. method, and (3) First order Born approximation. They have found that the first order Born approximation is not so good as the other two. It is with a view to seeing whether second Born approximation improves the theoretical findings we have done the calculation both for scattering as well as for polarization effects when electrons of energy 121 kev impinge on gold atom.

Mohr and Tassie (1954) have calculated the differential cross section and polarization effects of electrons scattered by gold by a semi-analytic method. Without making rigorous calculations with Dirac equation, they have added the influence of spin as a correction by assuming that the difference in the phase values when spin is taken and neglected is the same for the coulomb and the screened coulomb.

Sherman and Nelson (1959) have obtained by numerical computation, scattering cross section and polarization asymmetry for electron scattering by gold using Dirac equation, but they have neglected the screening.

Very recently Lin (1964) has made numerical computation for scattering cross section and polarization of electrons of 121 kev energy by screened gold atom. According to his estimate, the error in the calculation is less than 1%. On comparing our results with those of Lin we find that the differential scattering cross section results calculated by second Born approximation method agrees fairly well with values obtained by numerical computations, specially for smaller angles; however, the second Born approximation is found to be inadequate for polarization results.

MATHEMATICAL FORMULATION

The Dirac equation for an electron of energy E, rest mass m, moving in the field ZeV of an atom may be written as

$$[E - ic\hbar(\boldsymbol{\alpha} \cdot \mathbf{grad}) + \beta mc^2]\psi = -Ze^2 V\psi$$

where $\boldsymbol{\alpha}$, β are the Dirac matrices and wave function ψ has the four-component column form.

If we operate on both sides of the above equation by

$$D = [E + ic\hbar(\boldsymbol{\alpha} \cdot \mathbf{grad}) - \beta mc^2]$$

we obtain

$$[\nabla^2 + k^2]\psi = -\frac{Ze^2}{c^2\hbar^2} DV\psi \qquad \ldots (1)$$

where

$$k^2 = \frac{1}{\hbar^2 c^2}[E^2 - m^2c^4]$$

We seek a solution of Eqn. (1) the asymptotic form of which is

$$\psi = ae^{i\mathbf{k}_0 \cdot \mathbf{r}} + u\frac{e^{ikr}}{r} \qquad \ldots (2)$$

$\mathbf{k}_0$ denotes propagation vector along the incident direction, $|\mathbf{k}_0|^2 = k^2$.

The first part represents the incident wave which consists of particles having an arbitrary spin direction. If the incident particles move in the Z direction, then a can be written in the form

$$\begin{pmatrix} \dfrac{-c\hbar kA}{E+mc^2} \\ \dfrac{c\hbar kB}{E+mc^2} \\ A \\ B \end{pmatrix}$$

where $\dfrac{-B}{A} = \cot\dfrac{\chi}{2}e^{iw}$, (χ, w) being the spherical polar angle of the arbitrary spin direction of the incident wave.

The current due to the incident wave depends on $|A|^2+|B|^2$, A, B being the 3rd and 4th element of a. In the same way the current due to the scattered wave depends on $|u_3|^2+|u_4|^2$.

The elastic scattering cross section is

$$\frac{d\sigma}{d\Omega} = \frac{|u_3|^2+|u_4|^2}{|A|^2+|B|^2}$$

If we choose $|A|^2+|B|^2 = 1$, the scattering cross section is

$$\frac{d\sigma}{d\Omega} = |u_3|^2+|u_4|^2 \qquad \dots \quad (3)$$

The scattered wave is evaluated by Born approximation upto second order. In view of the asymptotic condition (2) the differential equation (1) may be converted into the following integral equation :

$$\psi(r) = ae^{i\mathbf{k}_0\cdot\mathbf{r}} - \frac{Ze^2}{\hbar^2c^2}\int G(\mathbf{r},\mathbf{r}')\,D'V(r')\psi(r')d' \qquad \dots \quad (4)$$

where $\qquad G(\mathbf{r},\mathbf{r}') = -\dfrac{4\pi}{|\mathbf{r}-\mathbf{r}'|}e^{ik|\mathbf{r}-\mathbf{r}'|}$,

is the appropriate Green's function.

For the first Born approximation, we replace $\psi(r')$ in the above integral by incident unperturbed wave function, $ae^{i\mathbf{k}_0\cdot\mathbf{r}}$.

Thus as a first approximation, we obtain

$$\psi^I{}_{sc} = \frac{e^{ikr}}{r}u^I = \frac{e^{ikr}}{r}\,\frac{Ze^2}{c^2\hbar^2}\,\frac{1}{4\pi}\,(\mathbf{k}_1|\mathbf{V}|\mathbf{k}_0)(E-c\hbar\boldsymbol{\alpha}\cdot\mathbf{k}_1-\beta mc^2)a$$

$\mathbf{k}_1$ denotes propagation vector in the scattered direction, $|\mathbf{k}_1|^2 = k^2$.

On simplification we have

$$u^I = \begin{pmatrix} u^I{}_1 \\ u^I{}_2 \\ u^I{}_3 \\ u^I{}_4 \end{pmatrix} = \begin{pmatrix} \cdots\cdots\cdots \\ \cdots\cdots\cdots \\ Af_1 - Bg_1 e^{-i\varphi} \\ Bf_1 + Ag_1 e^{i\varphi} \end{pmatrix},$$

where
$$f_1 = \frac{Ze^2}{c^2\hbar^2}\frac{1}{4\pi}(\mathbf{k}_1|\mathbf{V}|\mathbf{k}_0)[(E-mc^2)\cos\theta+(E+mc^2)]$$

$$g_1 = \frac{Ze^2}{c^2\hbar^2}\frac{1}{4\pi}(\mathbf{k}_1|\mathbf{V}|\mathbf{k}_0)[(E-mc^2)\sin\theta]$$

$$a_1 = \frac{1}{4\pi}(\mathbf{k}_1|\mathbf{V}|\mathbf{k}_0) = \frac{1}{4\pi}\int e^{-ik_1\mathbf{r}}Ve^{i\mathbf{k}_0\mathbf{r}}d\tau.$$

For the second Born approximation, we iterate the above Eqn. (4) once again and obtain

$$\psi^{II}{}_{sc} = \frac{e^{ikr}}{r}u^{II}$$

$$= \frac{e^{ikr}}{r}\left(\frac{Ze^2}{c^2\hbar^2}\right)^2(E-c\hbar\boldsymbol{\alpha}\cdot\mathbf{k}_1+\beta mc^2)[(E-\beta mc^2)a_2-a_3\,\alpha\cdot(k_0+k_1)]a$$

Expressing the amplitude as a column matrix, we have

$$u^{II} = \begin{pmatrix} u^{II}{}_1 \\ u^{II}{}_2 \\ u^{II}{}_3 \\ u^{II}{}_4 \end{pmatrix} = \begin{pmatrix} \cdots\cdots\cdots \\ \cdots\cdots\cdots \\ Af_2 - Bg_2 e^{-i\varphi} \\ Bf_2 + Ag_2 e^{i\varphi} \end{pmatrix}$$

where f_2 and g_2 are given by

$$f_2 = \left(\frac{Ze^2}{c^2\hbar^2}\right)^2\left[\{(E-mc^2)^2\cos\theta+(E+mc^2)^2\}a_2+(E^2-m^2c^4)(1+\cos\theta)\frac{2a_3}{\hbar c}\right]$$

$$g_2 = \left(\frac{Ze^2}{c^2\hbar^2}\right)^2\left[(E-mc^2)^2\sin\theta\cdot a_2+(E^2-m^2c^4)\sin\theta\,\frac{2a_3}{\hbar c}\right]$$

where,
$$a_2 = \frac{1}{4\pi(2\pi)^3}\int_c \frac{(\mathbf{k}_1|\mathbf{V}|\mathbf{k})(\mathbf{k}|\mathbf{V}|k_0)\,d^3k.}{k^2-k_0{}^2}$$

$$a_3 = \frac{\hbar c}{4\pi(2\pi)^3}\int_c \frac{(\mathbf{k}_1|\mathbf{V}|\mathbf{k})[(\mathbf{k}_0+\mathbf{k}_1)\cdot\mathbf{k})](\mathbf{k}|\mathbf{V}|\mathbf{k}_0)}{|\mathbf{k}_0+\mathbf{k}_1|^2(\mathbf{k}^2-\mathbf{k}_0{}^2)}\,d^3k.$$

From Eqn. (3) the scattering cross section is given by

$$\frac{d\sigma}{d\Omega} = |f|^2 + |g|^2 + (fg^* - f^*g)(-AB^*e^{i\varphi} + A^*Be^{-i\varphi})$$

where, $\quad f = f_1 + f_2, \quad g = g_1 + g_2$

For scattering of an unpolarized beam, we have to average over all spin directions. Thus retaining terms upto the order $(Ze^2/\hbar c)^3$, we get the scattering crosssection as

$$\begin{aligned} \frac{d\sigma}{d\Omega} &= |f|^2 + |g|^2 \\ &= |f_1|^2 + |g_1|^2 + 2(f_1 \boldsymbol{Re} f_2 + g_1 \boldsymbol{Re} g_2) \\ &= \frac{d\sigma_1}{d\Omega} + \frac{d\sigma_2}{d\Omega} \end{aligned}$$

$d\sigma_1$ is the usual scattering cross section in first Born approximation and is given by

$$\frac{d\sigma_1}{d\Omega} = 4\left(\frac{Ze^2}{\hbar c}\right)^2 \left[\frac{1}{4\pi}(\mathbf{k}_1|\mathbf{V}|\mathbf{k}_0)\right]^2 k^2\cos^2\frac{\theta}{2}\left(1 + \frac{m^2c^2}{k^2\hbar^2}\sec^2\frac{\theta}{2}\right) \quad \dots \quad (5)$$

and $d\sigma_2$ is the additional contribution to scattering cross section from second Born approximation. $d\sigma_2$ is given by

$$\frac{d\sigma_2}{d\Omega} = 8\left(\frac{Ze^2}{\hbar c}\right)^3 \frac{1}{\hbar c}\left[\frac{1}{4\pi}(\mathbf{k}_1|\mathbf{V}|\mathbf{k}_0)\right] Ek^2\cos^2\frac{\theta}{2}$$

$$\left[\boldsymbol{Re}\,a_2 + \frac{1}{\hbar c}\boldsymbol{Re}(2a_3) + \frac{2m^2c^2}{k^2\hbar^2}\sec^2\frac{\theta}{2}\,\boldsymbol{Re}\,a_2\right] \quad \dots \quad (6)$$

The asymmetry after double scattering of an initial unpolarized beam is given by

$$2\delta = 2|D(\theta)|^2 \Big/ \left[\frac{d\sigma}{d\Omega}(\theta)\right]^2$$

where $D = (fg^* - f^*g)$

$$= 4mic^2\left(\frac{Ze^2}{\hbar c}\right)^3 \frac{1}{\hbar c}\frac{1}{4\pi}(\mathbf{k}_1|\mathbf{V}|\mathbf{k}_0)\,k^2\sin^2\theta\left[\boldsymbol{Im}\,a_2 - \boldsymbol{Im}\,\frac{2a_3}{\hbar c}\right] \quad \dots \quad (7)$$

neglecting $\left(\frac{Ze^2}{\hbar c}\right)^4$ and higher order terms.

Thus we find that for the calculation of scattering cross section we need the real parts of a_2 and a_3 and of the asymmetry factor, their imaginary parts.

The above expressions (5), (6) and (7) are derived for any general potential which tends to zero faster than $1/r$. Particularly, for the case of gold atom we take the form of the potential as

$$ZeV = \frac{Ze^2}{r} \left(\alpha_1 e^{-\lambda_1 r} + \alpha_2 e^{-\lambda_2} \right)$$

With this potential, the values of a_1, a_2 and a_3 take a simple form,

$$a_1 = \frac{\alpha_1}{4k^2 \sin^2 \frac{\theta}{2} + \lambda_1^2} + \frac{\alpha_2}{4k^2 \sin^2 \frac{\theta}{2} + \lambda_2^2}$$

$$a_2 = \frac{4\pi}{(2\pi)^3} \left[\frac{\alpha_1^2}{k^3} M_3(\lambda_1, \lambda_1) + \frac{2\alpha_1\alpha_2}{k^3} M_3(\lambda_1, \lambda_2) + \frac{\alpha_2^2}{k^3} M_3(\lambda_2, \lambda_2) \right]$$

$$a_3 = \frac{4\pi}{(2\pi)^3} \frac{\hbar c}{|\mathbf{k}_0 + \mathbf{k}_1|^2} \left[\frac{\alpha_1^2}{k^3} (2k^2 + \lambda_1^2) M_3(\lambda_1, \lambda_1) + \frac{\alpha_1\alpha_2}{k^3} (4k^2 + \lambda_1^2 + \lambda_2^2) M_3(\lambda_1, \lambda_2) \right.$$

$$+ \frac{\alpha_2^2}{k^3} (2k^2 + \lambda_2^2) M_3(\lambda_2, \lambda_2) + \frac{\alpha_1^2}{k} M_2(\lambda_1, \lambda_1)$$

$$\left. + \frac{\alpha_2^2}{k} M_2(\lambda_2, \lambda_2) + \frac{2\alpha_1\alpha_2}{k} M_2(\lambda_1, \lambda_2) - \alpha_1^2 I_1 - \alpha_1\alpha_2(I_1 + I_2) - \alpha_2^2 I_2 \right]$$

The values of real parts of M_3, M_2, I_1 and I_2 have been calculated by Lewis (1956); we have further extracted the imaginary parts of these expressions and a list of all of them is inserted in the appendix.

The scattering cross sections and asymmetry factors for coulomb field, may be easily deduced from the expression (5), (6) and (7), noting that $\alpha_1 = 1$, $\lambda_1 = 0$ and $\alpha_2 = 0$ for coulomb field. The results are found to be identical with the corresponding results in Dalitz's paper (1951).

RESULTS AND DISCUSSIONS

Numerical calculation has been made for the differential cross section and polarisation of electrons of energy 121 Kev scattered by gold atom. The values of the parameters occuring in the expression for the potential are, as given by Mohr and Tassie,

$$\alpha_1 = \frac{20}{79}, \quad \alpha_2 = \frac{59}{79}, \quad \lambda_1 = \frac{1.3}{a_0}, \quad \lambda_2 = \frac{6}{a_0}.$$

(a_0 being the first Bohr radius).

We have compared our results with those of Sherman and Nelson (1959) and Lin *et al* (1963,64). Sherman *et al*, have calculated the scattering cross section and the asymmetry factor for unscreened coulomb field of gold by numerical computation of a large number of phase shifts. Lin *et al.* have further included the effect of screening in his extensive numerical computation.

The Born series converges very slowly in the present case as $\left(\frac{Ze^2}{\hbar v}\right)$ is equal to 0.97. Therefore, though the present calculation has been extended upto second order, the third and higher order terms are of considerable importance. For scattering cross section the first term dominates over the higher order terms but for asymmetry the contribution from the first term is zero, whereas the second and higher order terms are nearly of the same order of magnitude. Hence the neglect of higher order terms, affects the polarization more seriously than it does the scattering cross section.

In Fig. 1 we give the results of our numerical calculation of scattering cross section together with those of Sherman *et al.* and of Lin *et al.* A comparison shows

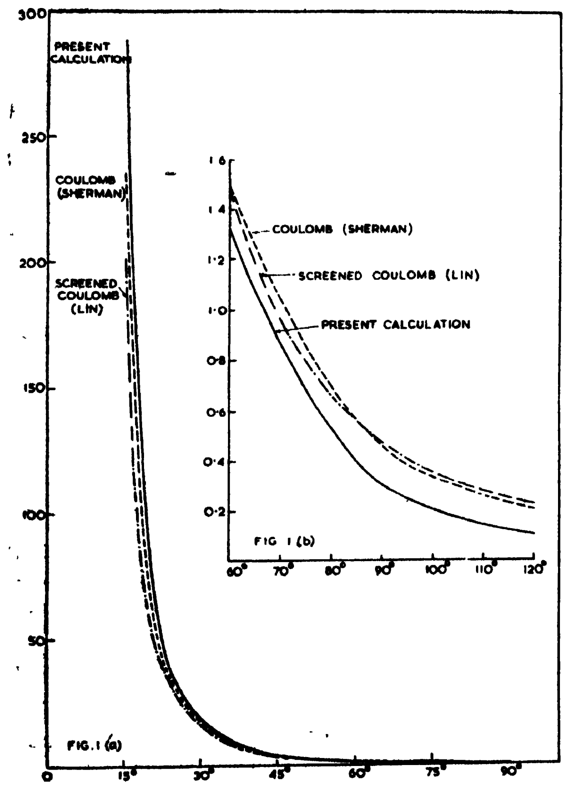

Fig. 1 (*a*) Differential scattering cross section in units of 10^{-20} cm.^{2}, against angle.
(*b*) The same with scales enlarged 100 times.

that the Born approximation gives fair agreement with the results of exact numerical calculations specially at small scattering angles, in the present case.

The numerical results for asymmetry in double scattering are shown in Figure 2.

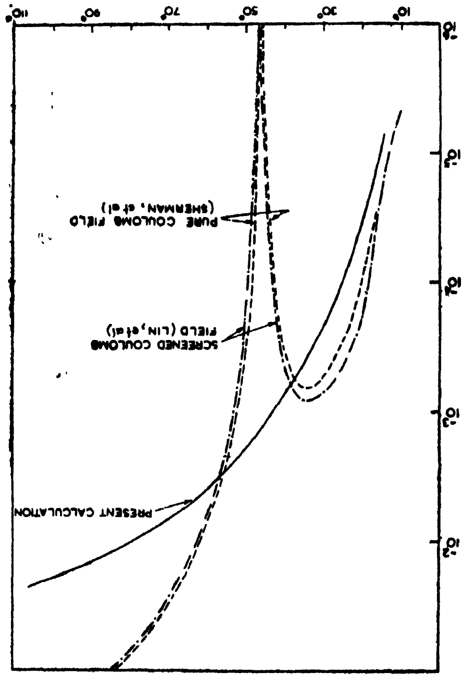

Fig. 2. The asymmetry $2\delta = 2 \dfrac{|D(\theta)|^2}{\left[\dfrac{d\sigma}{d\Omega}(\theta)\right]^2}$ after double scattring.

The value of the asymmetry after double scattering has a gradual tendency to increase with the increase of angles. The present calculation does not show the sudden fall in the asymmetry near 45° as observed by Sherman and Lin which according to them is due to the change of sign of the asymmetry factor.

It is to be noted that the accuracy of the method of calculation matters more than the inclusion of the screening effect. $fg^* - f^*g$ is so sensitive to small inaccuracies in the calculation of f and g that for a difference of 2% in the values of f and g leads to a difference of 15% in the assymetry factor, as has been remarked by Sherman.

The main source of error in the present calculation is the meglect of higher order terms in the Born series and it is expected that our analytical calculation will show a better agreement for elements of small atomic number in which case the higher order terms have less importance.

APPENDIX

The following values of M_3, M_2, I_1 and I_2 have been utilized in the calculation of a_2 and a_3 given in (3).

$$Re\ M_3(\mu, \nu) = \frac{\pi^2 k^3}{R}\left[\tan^{-1}\frac{S+R}{T} - \tan^{-1}\frac{S-R}{T}\right]$$

$$Im\ M_3(\mu, \nu) = \frac{\pi^2 k^3}{R}\ \tfrac{1}{2}\left[l_n\ \frac{T^2+(R+S)^2}{T^2+(R-S)^2}\right]$$

where,

$$R = [k^2(K^2+\mu^2+\nu^2)^2 - P^2\mu^2\nu^2]^{\frac{1}{2}}$$
$$S = k[K^2+(\mu+\nu)^2]$$
$$T = \mu\nu(\mu+\nu)$$
$$\mathbf{K} = \mathbf{k}_0 - \mathbf{k}_1$$
$$\mathbf{P} = \mathbf{k}_0 + \mathbf{k}_1$$

$$Re\ M_2(\mu, \nu) = \frac{2\pi^2 k}{|\mathbf{K}|}\ \tan^{-1}\ \frac{|\mathbf{K}|}{\mu+\nu}$$

$$Im\ M_2(\mu, \nu) = 0$$

$$Re\ I_i = \frac{\pi^2}{k}\ \tan^{-1}\frac{2k}{\lambda_i}$$

$$Im\ I_i = \frac{\pi^2}{k}\ l_n\ \frac{(4k^2+\lambda_i^2)^{\frac{1}{2}}}{\lambda_i}$$

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